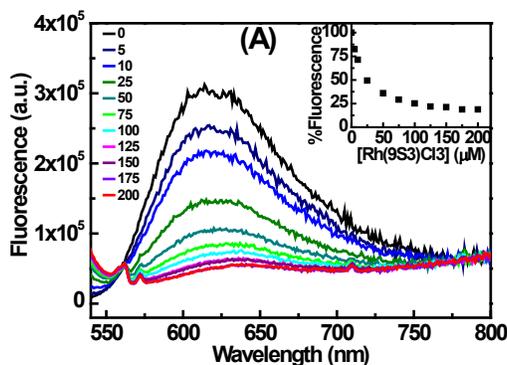


## Computational and Experimental Research Projects on Chemical Reactivity

Research Advisor: Dr. Titus V. Albu

### Experimental Project: *Fluorescence and UV-VIS Studies on Interaction of DNA with Thiosemicarbazones and Their Complexes*

The mechanism of action for some anticancer agents involves binding to DNA. Fluorescence techniques and UV-VIS spectroscopy will be used in this project to investigate the interaction between DNA and thiosemicarbazones or their complexes with transition metals. Carrying out an ethidium bromide (EB) displacement assay, the decrease in fluorescence emission will be monitored for samples containing DNA and EB in the absence and the presence of thiosemicarbazones or their complexes at various concentrations. This work is a collaborative project with Dr. Kim research group at UTC and Dr. Lisic group at Tennessee Tech University.



### Computational Project: *Hydrogen Abstraction from Fluorinated Compounds*

This project involves primarily the identification of transition states associated with different reaction pathways of hydrogen abstraction from hydrofluorocarbons and similar compounds. These reactions are relevant to the residence time in atmosphere for these compounds. The calculations will be carried out using Gaussian software on Linux workstations. This study will extend the current knowledge of reactivity of hydrofluorocarbons and similar compounds and will lead to a better understanding of the environmental impact of these industrially important compounds.

